

Supporting Information for:

**Response and Discrimination Performance of Arrays of Organothiol-Capped Au Nanoparticle Chemiresistive Chemical Vapor Sensors**

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**Table S1.** Resolution factors,  $rf$ , and performance values (parentheses) for all possible binary combinations of analytes tested at  $P/P^{\circ} = 0.0100$  by using the  $\Delta R_{\max}/R_b$  values; (a) discrimination values obtained for the R-SH Au-NP array; (b) discrimination values obtained for the R'-SH Au-NP array; (c) discrimination values obtained for the Ar-SH Au-NP array; d) discrimination values obtained for the C2Ph(Ar)-SH Au-NP array; e) discrimination values obtained for the combination of all sensor types studied.

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**Table S3.** Average resolution factor,  $\overline{rf}$ , obtained from the first five principal component variances captured, for each of the analyte vapors versus each polar group for five different sensor arrays; a) R-SH, b) R'-SH, c) Ar-SH, d) C2Ph(Ar) and e) all 20 sensors. The polar groups are divided into non polar vapors (R; Hex, Hept, Oct, *i*Oct, *c*Hex, Tol), polar aprotic vapors (R'; Chl, THF, EtOAc) and polar protic vapors (R-OH; MeOH, EtOH, *i*POH, BuOH),

a)	$\overline{rf}$	$\overline{rf}$ vs. R	$\overline{rf}$ vs. R'	$\overline{rf}$ vs. R-OH
Hex	30	1.0	5.1	85
Hept	13	0.94	2.7	35
Oct	8.7	1.0	2.1	23
<i>i</i> Oct	41	1.3	9.1	120
<i>c</i> Hex	43	2.2	8.4	120
Tol	11	0.79	3.5	31
Chl	13	11	7.8	17
THF	18	2.5	4.0	47
EtOAc	28	1.8	5.1	79
MeOH	94	140	89	3.5
EtOH	54	80	55	1.9
<i>i</i> POH	27	36	32	1.9
BuOH	13	16	15	2.6

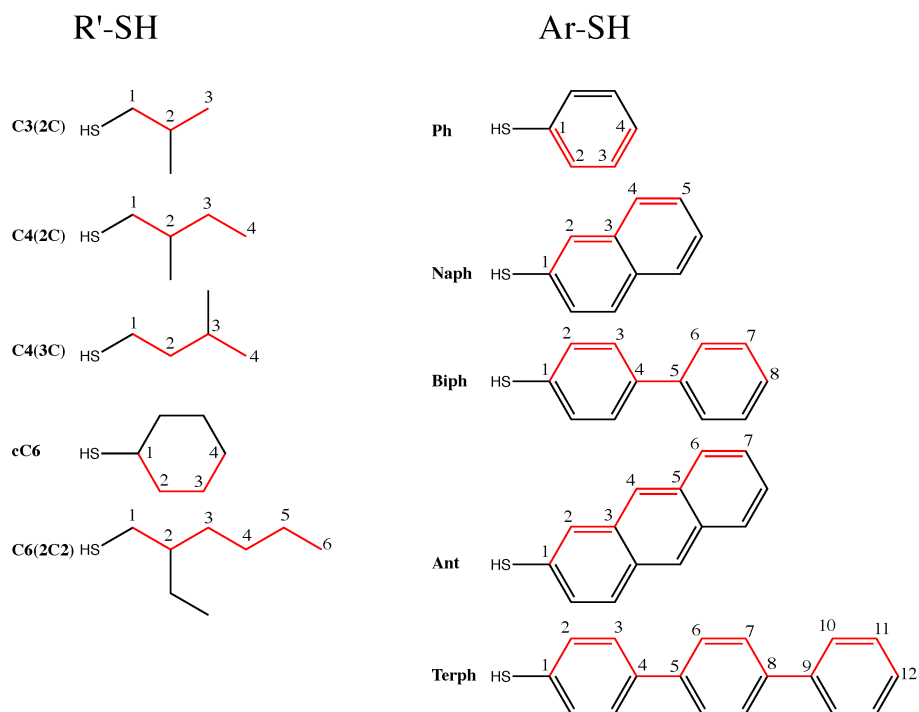
b)	$\overline{rf}$	$\overline{rf}$ vs. R	$\overline{rf}$ vs. R'	$\overline{rf}$ vs. R-OH
Hex	4.0	3.1	4.5	4.6
Hept	2.5	1.4	3.4	3.2
Oct	2.0	1.4	2.9	2.1
<i>i</i> Oct	5.6	1.8	11	6.2
<i>c</i> Hex	6.8	2.0	15	6.5
Tol	3.7	3.1	3.8	4.4
Chl	8.5	13	4.6	4.2
THF	3.8	4.5	3.8	2.6
EtOAc	3.9	3.3	5.6	3.8
MeOH	4.4	5.2	4.4	2.7
EtOH	4.2	5.3	3.3	2.9
<i>i</i> POH	2.8	3.5	2.5	1.8
BuOH	3.8	4.1	3.9	3.2

c)	$\overline{rf}$	$\overline{rf}$ vs. R	$\overline{rf}$ vs. R'	$\overline{rf}$ vs. R-OH
Hex	2.8	2.1	2.8	3.7
Hept	1.9	1.6	2.0	2.3
Oct	1.4	1.4	1.6	1.4
<i>i</i> Oct	5.3	2.1	9.8	6.0
<i>c</i> Hex	5.2	1.8	8.1	7.3
Tol	4.6	1.6	6.4	6.9
Chl	5.6	7.7	2.0	4.0
THF	3.6	4.5	2.8	2.6
EtOAc	2.9	3.1	2.0	2.9
MeOH	5.8	7.4	5.2	3.1
EtOH	5.8	8.4	3.7	2.6
<i>i</i> POH	1.5	1.4	1.3	2.2
BuOH	1.8	1.2	2.7	2.4

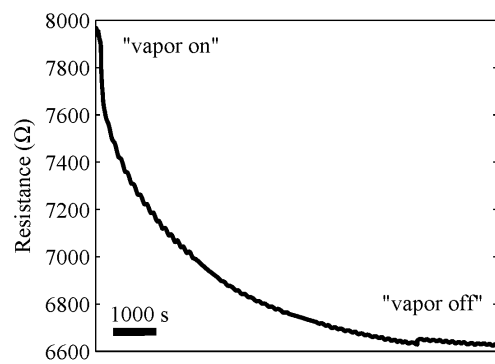


<b>d)</b>	$\overline{\sigma_f}$	$\overline{\sigma_f}$ vs. R	$\overline{\sigma_f}$ vs. R'	$\overline{\sigma_f}$ vs. R-OH
Hex	3.2	2.6	3.1	4.0
Hept	2.1	1.1	2.8	2.9
Oct	2.0	1.2	2.8	2.3
<i>i</i> Oct	6.3	1.8	13	7.4
<i>c</i> Hex	4.8	1.7	8.2	6.2
Tol	3.9	1.3	6.6	5.2
Chl	6.8	9.8	4.7	3.3
THF	5.2	6.8	3.6	3.5
EtOAc	2.6	1.4	4.8	3.2
MeOH	4.4	5.9	4.4	1.5
EtOH	3.0	3.0	3.9	1.9
<i>i</i> POH	3.2	4.4	2.7	1.5
BuOH	3.9	5.5	2.4	2.2

<b>e)</b>	$\overline{\sigma_f}$	$\overline{\sigma_f}$ vs. R	$\overline{\sigma_f}$ vs. R'	$\overline{\sigma_f}$ vs. R-OH
Hex	8.3	4.0	7.1	15
Hept	5.5	2.6	3.9	10
Oct	4.7	2.0	4.1	8.7
<i>i</i> Oct	10	3.3	17	14
<i>c</i> Hex	10	2.9	16	15
Tol	6.3	2.9	6.9	10
Chl	12	14	9.1	12
THF	9.4	8.5	7.1	12
EtOAc	7.5	5.4	8.2	10
MeOH	11	13	14	4.5
EtOH	11	15	10	3.5
<i>i</i> POH	8.8	10	11	3.5
BuOH	7.8	9.7	8.9	3.0



**Figure S1.** Molecular structure and chain length determination of the R-SH and Ar-SH organothiol ligands. The red-labeled bonds represent the atoms/bonds considered for the chain length determination, where the highest number represent the value of chain length.



**Figure S2.** Resistance response of a Au-C5 chemiresistive sensor upon exposure to saturated ethanol vapor.